

# Cyclohexylhemicucurbit[8]uril – A Chiral Macrocyclic Host for Anionic Guests

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Cucurbituril chemistry has gained considerable interest over the last decades. Classical cucurbit[*n*]uril (CB[*n*]) homologues, known to encapsulate neutral or positively charged molecules, have already been employed in stimuli responsive systems and in CB[*n*] mediated catalysis.<sup>1,2</sup> Accounts of anion binding within CB[*n*] homologues are scarce, with the exception of hemicucurbit[*n*]urils (HC[*n*]), a sub-group of the CB[*n*] family, known to preferentially bind anions.<sup>3,4</sup>

Chiral cyclohexylhemicucurbit[*n*]urils (cycHC[6]) have been synthesized and investigated by our group.<sup>5,6</sup> The electron-poor cavity of cycHC[*n*] renders these macrocycles capable of anion recognition.<sup>7</sup> Our recent efforts to gain insight into the binding of anionic guests by cycHC[8] have resulted in a number of successfully crystallized and structurally characterized complexes. Crystal structures of 1:1 complexes with a number of singly charged tetrahedral and octahedral anions have been successfully obtained, demonstrating the remarkable ability of cycHC[8] to accommodate guests of different shapes and sizes. The flexible nature of the cycHC[8] portals allows for tight sealing of the encapsulated guests. Additionally, the binding of anionic guests to cycHC[8] has been complementarily evaluated by ESI-TOF MS and NMR spectroscopy.

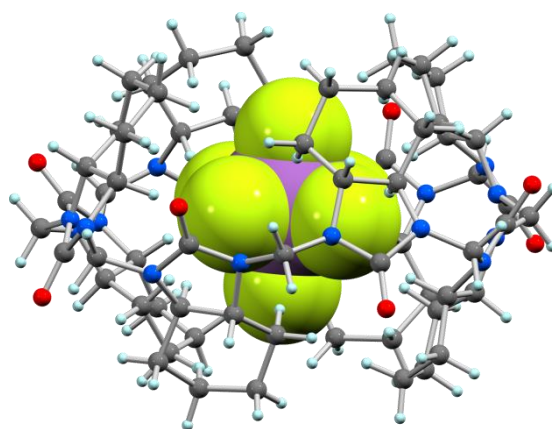


Figure 1: The structure of an inclusion complex of cycHC[8]:SbF<sub>6</sub><sup>-</sup> from X-ray diffraction analysis

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